

# Modelling of the process of burning coke on catalyst grain

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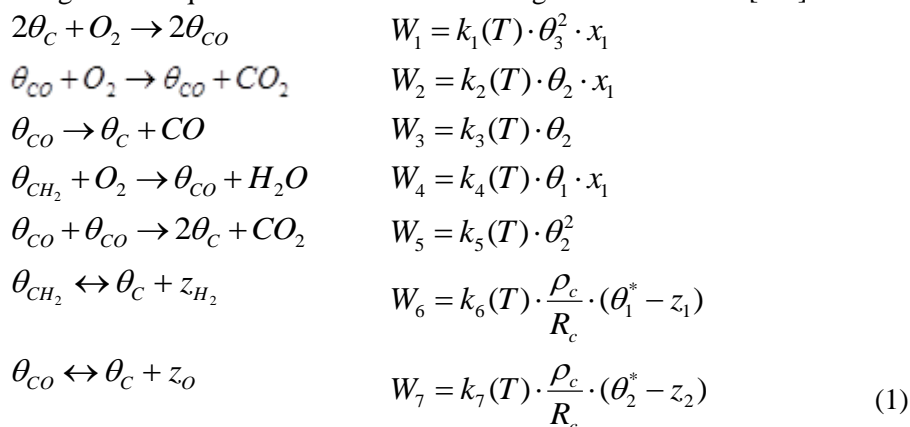
**Abstract.** Based on the kinetic model of oxidative regeneration of coked catalysts, a two phases diffusion mathematical model of the process of oxidative regeneration of coked catalysts in a catalyst grain has been enhanced. A numerical analysis of the heating on the grain was carried out over a wide range of the initial oxygen concentration, inlet temperature, and gas flow velocity. It is established that the process of burning coke has a high parametric sensitivity to the initial oxygen concentration.

## 1. Introduction

Against the background of economic sanctions from foreign manufacturers, research on restoring the activity of coked catalysts becomes urgent. The most common technological method is the burning of coke deposits with oxygen-containing air. The process of burning coke deposits is non-stationary, and often, due to large thermal casts, dangerous, abnormal situations arise. It is necessary to determine the possible maximum preheat for different initial coke deposits. It is not economically profitable and sometimes dangerous to carry out special experiments on factory settings. Therefore, computer simulations are used to assess possible heating.

## 2. The scheme of chemical transformations

The scheme of chemical transformations describing the oxidation of coke deposits of some averaged formula, and the corresponding kinetic equations of the rates of the stages have the form [1-3]:



where  $W_i$  speeds of individual stages  $\frac{moth}{m^2 \cdot s}$  for  $W_1 - W_5$  и  $\frac{g}{m^2 \cdot s}$  for  $W_6 - W_7$ ;  $k_1(T)$  temperature-dependent rate constants ( $T$ ) according to the Arrhenius equation (dimension).

$k_2(T)$  matches the dimension  $W_i$ ), the values of the constants are given in the table 1;  $x_i$  - oxygen concentration in the gas phase, molar fractions;  $z_i$  - hydrogen concentration ( $z_1 = z_{H_2}$ ) and oxygen ( $z_2 = z_O$ ) in the volume of coke deposits,  $\frac{g}{g}$ ;  $\theta_k$  - degrees of coke surface coverage with various carbon complexes ( $\theta_1 = \theta_{CH_2}$ ) - hydrogen-carbon complex,  $\theta_2 = \theta_{CO}$  - oxygen-carbon complex,  $\theta_3 = \theta_C$  - free carbon surface);  $\theta_k^*$  - amount of coke adsorbed by hydrogen ( $k = 1$ ) and oxygen ( $k = 2$ ) equilibrium relative to the current state of the surface of the coke deposits,  $\frac{g}{g}$ ;  $\rho_c$  - coke density  $\frac{g}{m^3}$ ;  $R_c$  - average radius of coke pellets, m.

Oxidative regeneration is a non-stationary process, because the amount of coke on the catalyst decreases during burning. This is accompanied by continuous restructuring of the outer surface and a change in the composition of coke deposits over time. ( $\bar{z}$ ) due to the exchange surface - the volume of coke pellets. Coke can be considered as a chemical compound of some averaged formula  $CH_n$  or  $CH_nS_m$ , the main combustible component is carbon. Therefore, the coke content on the catalyst ( $q_c$ ) extracted from vector  $\bar{z}$ , and the concentrations of the remaining components of this vector are calculated relative to  $q_c$ . Then the change in the composition of coke deposits on the catalyst is described by the following material balance equations:

$$\begin{aligned} \frac{dq_c}{dt} &= M_c S_k \sum_{j=1}^J v_{1j} W_j; \\ \frac{d(z_n q_c)}{dt} &= S_k \sum_{j=1}^J v_{nj} W_j, \quad n = \overline{2, N}; \end{aligned} \tag{2}$$

with initial conditions -  $q_c = q_c^o, z_n = z_n^o$ ; where  $t$  - is time, c;  $M_c$  - coke molecular weight  $\frac{g}{moth}$ ;  $S_k$  coke pellet specific surface,  $\frac{m^2}{g_{ct}}$ ;  $q_c^o$  - initial coke content  $\frac{g}{g_{ct}}$ ,  $N$  - the amount of bulk components.

**Table 1.** Constants of the kinetic model (1) for an aluminosilicate catalytic cracking catalyst [2, 3].

$\widehat{K}_i$	$\widehat{K}_i(520^\circ\text{C}), c^{-1}$	$E_i, \text{kJ/moth}$	$\widehat{K}_i$	$\widehat{K}_i(520^\circ\text{C}), c^{-1}$	$E_i, \text{kJ/moth}$
$\widehat{K}_1$	0,112	99,1	$\widehat{K}_5$	1,890	27,3
$\widehat{K}_2$	0,563	90,8	$\widehat{K}_6$	5,923	154,5
$\widehat{K}_3$	0,220	52,8	$\widehat{K}_7$	1,890	42,7
$\widehat{K}_4$	0,315	50,4			

To estimate the heating of the catalyst grain using the mathematical description (2), calculations were done, the results of which are presented in the form of dependences in Fig. 1 (a-г). As a basic selection, the following set of parameters:  $q_c^o = 5\%$  (mas.),  $x_1^o = 2,0\%$  (vo.),  $T = 500^\circ\text{C}$ ,  $d_3 = 5$  mm. In the calculations, one of the parameters was varied at constant values of the other three.

Interesting dependence of the maximum heat  $\Delta T$  from inlet temperature  $T_0$  - characteristic S-figurative curve emerging with an increase in temperature on the asymptotic line. A similar curve is obtained for the dependence  $\Delta T$  on oxygen concentration  $x_1^0$ , however parametric sensitivity ( $\Delta T$  from  $x_1^0$ ) higher than for ( $\Delta T$  from  $T^0$ ). Although this result is characteristic of liquid-phase combustion processes with a high liquid [4, 5, 6, 7, 8] the combustion of a condensed medium (coke) once again confirms the thermodynamic generality of combustion problems.

### 3. References

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